Development of a new phosphatidylcholine-like surfactant and its application in cosmetics

Poster ID

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Introduction:

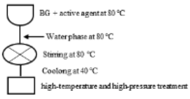
In cosmetics, surfactants are important components that significantly contribute not only to the functionality and feeling of use of commodities but also to their stability.
Conventional surfactants used in cosmetics are monomeric; however, attention has been focused in recent years on a gemini surfactants, in which are tethered to each other in the vicinity of a hydrophilic group by an appropriate linking group. Gemini-type surfactants have an extremely low critical micelle concentration (CMC), high interfacial tension-lowering ability, and high surfactant ability, which is represented by a low kraft point. In addition, they exhibit excellent characteristics such as high molecular associativity, antibacterial, high foaming and penetration properties, which enable the spontaneous formation of higher-order structures such as vesicles (*2). Gemini-type surfactants are capable of expressing a surfactant scientific function equivalent to or higher than that of single-chain single hydrophilic group surfactants with a small addition amount ; by replacing a conventional surfactant with a gemini surfactant, the total amount of surfactant used can be reduced, thereby resulting in low environmental load.
Meanwhile, phospholipids are constituents of biological membranes; thus, they are used in many cosmetics as surfactants with high safety. Phosphocholine (PC) groups, which are polar groups of phospholipids that exhibit excellent characteristics such as biocompatibility and moisture retention, are widely utilized as functional groups.
Therefore, we aimed to develop novel surfactants with high safety and biocompatibility similar to those of phospholipids and gemini-type activators. Therefore, we focused on phosphatidylcholine, a phospholipid, and [PCG(P(18)-N(22))], a gemini-type active agent with a phosphocholine group, to develop a new surfactant and determine its functionality

Materials & Methods:

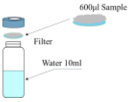
Materials
1.3-Butylene glycol (BG), phospholipids, [PCG(P(18)-N(22))], [PCG(P(22)-N(Et)(18:1))], [PCG(P(18:1)-N(Et)(22))], glyceryl tri-2-ethylhexanoate, isoparaffin, vaseline, purified water, carrageenan sucrose mixture, and PEG phytosterol.

Solubility Test
0.25 g of each sample into a beaker and add 24.75 g of each liquid component (1% sample concentration). Then, heat to 70 ℃.

Sample preparation



Water Evapotranspiration Measurement
600 μl of the prepared sample was dropped onto a filter, dried, placed in a vial containing 10 ml of purified water, and the amount of water evaporation was measured over time at 40 ℃.



Evaluation
・Small-angle X-ray scattering measurements (SAXS) :
・Dynamic light scattering (DLS)
・Transmission electron microscopy (TEM)
・Observed of Maltese cross: The prepared samples observed by polarized light microscopy were used to confirm the Maltese cross via modified electron microscopy

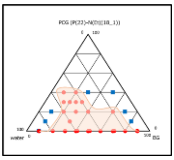
Results & Discussion:

Sample selection
With their unsaturated bonds and hydroxyethyl groups, [PCG(P(22)-N(Et)(18:1))] and [PCG(P(18:1)-N(Et)(22))] exhibit high interfacial tension-lowering ability and emulsification stability(*1). Therefore, their solubility and emulsification maintenance time in polar and hydrocarbon oils, which are general-purpose materials in cosmetics, were confirmed (Table 1) .Based on their solubility and emulsification maintenance time, [PCG(P(22)-N(Et)(18:1))] showed excellent solubility and emulsification maintenance time in polar and hydrocarbon oils; thus, [PCG(P(22)-N(Et)(18:1))] was selected for use in this study.

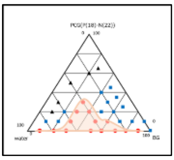
	Solubility			Emulsification maintenance time	
Surfactant	Polar oil	Hydrocarbon oil	Water	Polar oil	Hydrocarbon oil
PCG(P(18)-N(22))	△	×	×	**15 min**	×
PCG(P(22)-N(Et)(18:1))	○	○	×	**60 min**	**45 min**
PCG(P(18:1)-N(Et)(12))	△	×	×	×	**Not soluble**

Table1

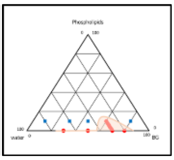
Fabrication of three-phase diagrams
[PCG(P(18)-N(22))] Based on vesicle formation, [PCG(P(22)-N(Et)(18:1))] may form associates as well. Therefore, we confirmed the changes in the regions in each phospholipid, [PCG(P(18)-N(22))], [PCG(P(22)-N(Et)(18:1))], which can confirm the association with optical anisotropy (Maltese cross confirmation). This was confirmed by fabricating three-phase diagrams using 1, 3-BG, water, and various surfactants (Figures 1-1 to 1-3). Each site (plot) was color-coded according to Maltese cross confirmation and appearance of the samples(Table 2). The results show that the regions where liquid and Maltese crosses were identified were larger in [PCG(P(22)-N(Et)(18:1))] compared to those in phospholipids and [PCG(P(18)-N(22))]. In addition, [PCG(P(22)-N(Et)(18:1))] can confirm the Maltese cross in the low concentration region, where the Maltese cross cannot be confirmed with phospholipids and [PCG(P(18)-N(22))]. This reveals that compared to phospholipids and [PCG(P(18)-N(22))], [PCG(P(22)-N(Et)(18:1))] has a wider region to form associates with optical anisotropy.



Figures 1-1



Figures 1-2



Figures 1-3

	Condition
▲	Not soluble
■	Solid state
●	Liquid state

Table2

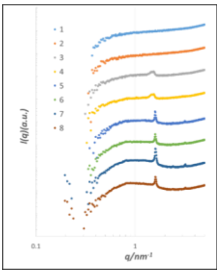
Analysis of associates
[PCG(P(22)-N(Et)(18:1))] To analyze the physicochemical properties of the formed associates, samples according to the following formulations (Tables 3-1, 3-2) were prepared and analyzed by DLS, SAXS, and TEM. The result of DLS and SAXS of the prepared samples are shown in (Figures 2-1 and 2-2). To confirm the effect of other factors on the associates, samples were prepared by mixing water-soluble polymers and high-pressure treatment. The samples were also analyzed by DLS and SAXS measurements (Figures 3-1, 3-2). Additional TEM observations were also conducted, and multilayered associates were observed (Figure 4). These results suggested that the associate formed by [PCG(P(22)-N(Et)(18:1))] was a vesicle.

	1	2	3	4	5	6
PCG(P(22)-N(Et)(18:1))	0.01	0.01	0.1	0.1	1	1
1, 3-BG	31	31	31	31	31	31
Water	68.99	68.99	68.8	68.8	67	67
PEG-Phytosterol	—	—	0.1	0.1	1	1
carrageenan sucrose mixture	—	—	—	—	—	—
High-pressure treatment	—	2	—	2	—	2
Warming High-pressure treatment	—	—	—	—	—	—

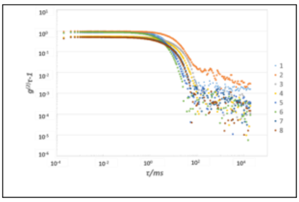
Table3-1

	7	8	9	10	11
PCG(P(22)-N(Et)(18:1))	0.5	0.5	0.5	1	2
1, 3-BG	31	31	36	36	36
Water	68	68	62.75	61.75	59.75
PEG-Phytosterol	0.5	0.5	0.5	1	2
carrageenan sucrose mixture	—	—	0.25	0.25	0.25
High-pressure treatment	—	2	—	—	—
Warming High-pressure treatment	—	—	2	2	2

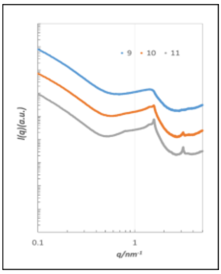
Table3-2



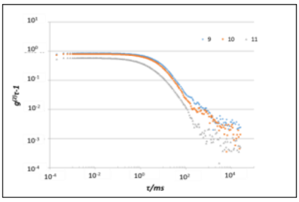
Figures 2-1



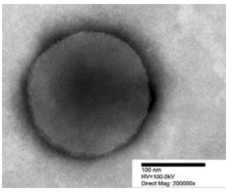
Figures 2-2



Figures 3-1



Figures 3-2

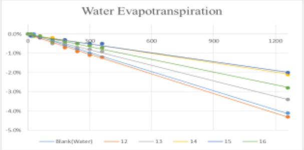


Figures 4

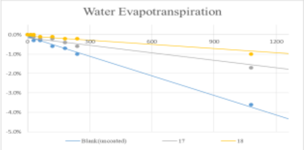
Water Evapotranspiration Measurement
[PCG(P(18)-N(22))] showed significant results in the water retention test(*2), [PCG(P(22)-N(Et)(18:1))] may have the same moisture retention capacity. Therefore, a moisture evaporation measurement test was conducted using samples prepared with the following formulation (table 4). The results are shown below (Figure 5-1). The results showed [PCG(P(22)-N(Et)(18:1))] was as effective as [PCG(P(18)-N(22))] in inhibiting water evaporation. [PCG(P(22)-N(Et)(18:1))] + Isoparaffin and [PCG(P(22)-N(Et)(18:1))] + Vaseline were also found to be more effective in inhibiting water transpiration compared to no application. (Figure 5-2).

	12	13	14	15	16	17	18
PCG(P(22)-N(Et)(18:1))	—	0.5	0.5	—	—	0.5	0.5
PCG(P(18)-N(22))	—	—	—	0.5	—	—	—
Phospholipids	—	—	—	—	0.5	—	—
1, 3-BG	36	36	36	36	36	36	36
Water	62.75	62.75	62.75	62.75	62.75	61.75	61.75
PEG-Phytosterol	0.5	0.5	0.5	0.5	0.5	0.5	0.5
Isoparaffin	—	—	—	—	—	1	—
Vaseline	—	—	—	—	—	—	1
carrageenan sucrose mixture	0.25	—	0.25	0.25	0.25	0.25	0.25
Warming High-pressure treatment	2	2	2	2	2	2	2

Table 4



Figures 5-1



Figures 5-2

Discussion
The ability of [PCG(P(22)-N(Et)(18:1))] to form associates was higher than that of phospholipids [PCG(P(18)-N(22))]. This superior ability may be attributed to the critical packing parameter (R) of [PCG(P(22)-N(Et)(18:1))], which indicates that it is more likely to form an associate. Moreover, DLS measurement of the sample was conducted by compounding the water-soluble polymer, and the SAXS results proved that the SAXS profile changed in the sample blended with the water-soluble polymer. This result may be attributed to the change in structure of the associate contained within the original sample caused by the addition of the water-soluble polymer. Thus, the combination of the water-soluble polymer and [PCG(P(22)-N(Et)(18:1))] may have formed a new associate different from the original associate.

Conclusions:

A new gemini-type surfactant was developed, and its functionality was determined. The association formed by [PCG(P(22)-N(Et)(18:1))] was confirmed to be a vesicle. Moreover, the new surfactant showed improved vesicle formation ability compared to those of phospholipids and [PCG(P(18)-N(22))]. Further, [PCG(P(22)-N(Et)(18:1))] was as effective as [PCG(P(18)-N(22))] in inhibiting water evaporation. In short, cosmetics prepared using [PCG(P(22)-N(Et)(18:1))] are considered to have high functionality. The vesicles formed by [PCG(P(22)-N(Et)(18:1))] are expected to be highly effective in Transepidermal Water Loss(TEWL) and stratum corneum water content. In the future, further detailed analysis of associates and their usefulness on the skin will be conducted.

References:

(*1) Ayami Kobayashi et al., 60th Annual Society of the Japan Oil Chemistry Society (2021)
(*2) H. Okawa, K. Hanabusa, M. Suzuki, H. Fukui, Efficacies of a novel Gemini Compound "2-(Dimethyldocosylammonio)ethyl octadecyl ethyl phosphate" as a Cosmetic ingredient, International Journal of Research in Cosmetic Science, 3(2) (2013) 19-24.